

**National Exposure Research Laboratory
Research Abstract**

Government Performance Results Act (GPRA) Goal 1
Annual Performance Measure 222

Significant Research Findings:

Science Version of PM Chemistry Model

**Scientific
Problem and
Policy Issues**

Results of peer reviewed studies conducted over the past decade demonstrate elevated levels of particular matter (PM) containing a complex mixture of inorganic and organic compounds reduce visibility, affect climate change, and adversely impact human health. In those areas of the United States where ambient PM_{2.5} (fine PM less than 2.5 micrometers in diameter) concentrations exceed the National Ambient Air Quality Standards (NAAQS), State Implementation Plans (SIPs), which include emission control strategies, must be developed and submitted to EPA. The control strategies rely on air quality models to assess the change in ambient levels for a specific reduction in emission rates of PM_{2.5} and its precursors. The reliability of the air quality predictions depends on the accuracy of the model descriptions of the formation and fate of PM_{2.5}.

The chemistry of PM_{2.5} is determined by of hundreds of inorganic and organic compounds spread across solid and liquid phases, all of which may interact with each other. Although many of these compounds are directly emitted into the atmosphere from stationary stacks and motor vehicles, some are formed from reactions of the primary gas phase emissions. The atmospheric chemistry of such secondary formation is reasonably well established for the inorganic compounds forming PM_{2.5} (i.e., NO_x and SO₂). Only recently have methods been developed for predicting ambient concentrations of organic PM_{2.5} compounds formed by secondary processes, and no PM chemistry model has been developed that adequately treats secondary formation of both inorganic and organic fractions.

**Research
Approach**

The objective of this research is to develop a PM chemistry model that includes a secondary organic PM formation module. For the past six years, EPA's National Exposure Research Laboratory (NERL) has been conducting laboratory and field studies to understand key chemical processes controlling ambient PM_{2.5} compositions and concentrations, with emphasis on determining those processes involving organic compounds. EPA/NERL conducted studies to identify major chemical processes affecting secondary contributions to PM_{2.5} concentrations by organic compounds emitted from motor vehicle exhaust and vegetation, two sources thought to contribute significantly to the organic fraction of ambient PM_{2.5}. EPA/NERL and its research partners have used computational chemistry-based methods for predicting thermodynamic properties of organic compounds, thus providing critical input data for the PM chemistry model. This information, along with data from the peer-reviewed literature, has been used to expand the Aerosol Inorganics Model (AIM), developed by Dr. Simon Clegg of the University of East

Anglia and Professor Anthony Wexler of the University of California at Davis, to include organic compounds, thus creating the Aerosol Inorganics and Organics Model (AIOM), a PM chemistry model for predicting compositions and concentrations of real-world PM_{2.5}.

Results and Impact

The AIOM contains advanced treatments of the key inorganic and organic chemical processes that control ambient PM_{2.5} concentrations and compositions. The inorganic component of the model, the AIM, has been used and tested extensively and is generally accepted in the atmospheric chemistry community as the most advanced inorganic chemistry model available. The expansion of the AIM to include organic-organic and inorganic-organic interactions has made it possible to predict ambient concentrations of *both* inorganic and organic compounds.

The execution time of the AIOM is still too long for it to be incorporated into air quality models for routine use. Model simplification and comparison of model outputs with laboratory and field data is needed to produce a tool that can be used by EPA and the States to calculate real-world ambient PM_{2.5} concentrations. The simplified model will be used to develop general control strategies for meeting the mass-based PM_{2.5} NAAQS, and to develop specific control strategies for reducing ambient concentrations of those PM_{2.5} compounds responsible for adverse health effects. The AIOM will also be used to calculate the relative contributions of primary and secondary emissions to ambient PM_{2.5} concentrations and the relative contributions of biogenic and anthropogenic sources to PM_{2.5} concentrations, and to assess the impact of reductions of SO₂ emissions on PM_{2.5} nitrate concentrations.

Research Collaboration and Research Products

The laboratory and field study research was carried out by the NERL Atmospheric Chemistry Research Team that consists of Drs. Edward Edney, Tadeusz Kleindienst, Michael Lewandowski and John Offenberger, with onsite technical support from Dr. Mohammed Jaoui and Eric Corse of ManTech Environmental Technology, Inc. The development and initial evaluation of the science version of the AIOM was carried out by Dr. Simon Clegg of the University of East Anglia with input from Dr. Edward Edney and Professor Libero Bartolotti of East Carolina University.

Examples of recent publications from this study include:

Edney, E.O. and Clegg, S.L. "Extension of the Aerosol Inorganics Model to Include Organic Compounds with User-Defined Properties." To be submitted to Journal of Aerosol Science 2004.

Kleindienst, T.E., Jaoui, M., Lewandowski, M., and Edney, E.O. "Identification and Quantification of Aerosol Polar Oxygenated Compounds Bearing Carboxylic and/or Hydroxyl Groups 1. Method Development." Analytical Chemistry (In Press) 2004.

Kleindienst, T.E., Conner, T.S., McIver, C.D., and Edney, E.O. "Determination of Secondary Organic Aerosol Products from the Photooxidation of Toluene and their Implications in Ambient PM_{2.5}." Journal of Atmospheric Chemistry 47:79-100, 2004.

Edney, E.O., Kleindienst, T.E., Conner, T.S., McIver, C.D., Corse, E.W., and Weathers, W.E. "Polar Organic Oxygenates in PM_{2.5} at a Southeastern Site in the United States." Atmospheric Environment 37:3947-3965, 2003.

Edney, E.O., Clegg, S.L., L.J. Bartolotti, and Kleindienst, T.E. "Computational Chemistry Method for Predicting Vapor Pressures and Activity Coefficients of Polar Organic Compounds in PM_{2.5}" Presented at the 21st Annual Conference of the American Association of Aerosol Research Charlotte, NC October, 2002.

Future Research

To date, more than 5,000 simulations have been conducted to evaluate the numerical accuracy of the new AIOM code. In addition, two of EPA/NERL's leading aerosol chemistry modelers have reviewed the model, and efforts are underway to compare the AIOM predictions with those of the existing PM chemistry models. Further research will include comparing model predictions of the AIOM with laboratory and field data, and simplifying the model and subjecting it to critical review so that it can be integrated into EPA air quality models.

**Contacts for
Additional
Information**

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